

Model Performance

Model	Data
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Weighted KNN model					
5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 295 °C

Global applicability domain: Outside

Local applicability domain index: 4.34e-02

Confidence level: 8.04e-01

Nearest Neighbors from the Training Set

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<div>Image not found</div> <div>Diphenylurea</div> <div>Measured: 262</div> <div>Predicted: 269</div>	<div>Image not found</div> <div>N-(4-Bromophenyl)urea</div> <div>Measured: 260</div> <div>Predicted: 256</div>	